Theory of spin-dependent conductivity in GMR materials

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This paper presents a critical review of theoretical studies of spin-dependent conductivity in GMR (giant magnetoresistive) materials. Earlier studies used relatively simple models of the electronic states and energy-band structure. Several more recent calculations of electronic transport in layered materials are based on *ab initio* treatment of the spin-dependent energy bands and Fermi surface. By including realistic energy-band structures, these studies have been able to make quantitative comparisons of alternative mechanisms for enhanced magnetoresistance and to explain the relative importance of spin-dependent scattering at interfaces.

1. Introduction

Giant magnetoresistance (GMR) was first observed in layered Fe/Cr magnetic structures by Baibich et al. [1] and by Binasch et al. [2]. These structures have magnetized layers separated by a nonmagnetic spacer metal.

A material with magnetized layers or granules that is spontaneously antiferromagnetic, or whose magnetization vectors are randomly oriented, exhibits GMR when the electrical resistivity is significantly reduced by a magnetic field that induces parallel magnetization alignment. GMR is characterized by the magnetoresistance ratio $\Delta R/R$, where ΔR is the total decrease of electrical resistance as the applied magnetic field is increased to saturation and R is measured in the state of parallel magnetization. The underlying physical process in GMR materials is dissipative scattering that is stronger for one spin component of the electronic current density, depending on magnetization. If the spin polarization of the electrons is well-defined on a length scale that is large compared with the spacing of magnetized layers or granules, both spin components are relatively strongly scattered when local magnetization directions vary. If the magnetization vectors are ferromagnetically aligned, the more weakly scattered spin component carries electric current with lower resistivity and shunts out the more strongly scattered component.

Although the original experiments were done with nearly perfect crystalline films produced by molecular beam epitaxy (MBE), Parkin et al. [3] showed that GMR occurs in metallic films deposited by sputtering, allowing much simpler fabrication. An experimental survey of GMR for Co/Ru, Co/Cr, and Fe/Cr sputtered superlattice structures revealed that the saturation magnetoresistance oscillates with spacer layer thickness [3]. This has turned out to be due to oscillation of the interlayer exchange coupling between magnetized layers, which is not discussed here. If antiparallel alignment is forced on the initial structure, the GMR ratio simply decreases monotonically with spacer thickness [4]. Another result discovered using sputtered samples is that Co/Cu layered structures have large room-temperature GMR ratios if the Cu spacer thickness is chosen to make the oscillatory exchange coupling between Co layers antiferromagnetic [5, 6].

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While GMR was originally observed for layered elemental metals, it was found to occur for ferromagnetic permalloy ($Ni_{80}Fe_{20}$) [7] and also for granular materials [8]. In the case of permalloy (Py), the magnetoresistance ratio is reduced by compositional intermixing at Py/Cu interfaces [9]. This is attributed to reduction of magnetization in the mixed layers. An inverse GMR effect is observed if thin Cr layers are intercalated into Fe in an Fe/Cu multilayer structure [10].

In a series of experiments designed to probe the relative effect of interface and bulk scattering in GMR materials, Parkin [11] showed for many different combinations of metals that the magnetoresistance depends exponentially on the thickness of an interface layer, with a characteristic length that is extremely short. These experiments were done with sputtered spin-valve structures described as exchange-biased sandwiches (EBS), of the form $F_1/S/F_2$/FeMn. The magnetization of layer F_2 is pinned by exchange coupling to antiferromagnetic FeMn, and the magnetization of layer F_1 is controlled by the applied magnetic field. In the principal experiment, metals F_1 and F_2 were permalloy (Py) and the spacer S was Cu. Very thin layers of Co were deposited at the Py/Cu interfaces. These layers produced a large increase in the GMR ratio, which approaches a saturation value on a length scale of atomic size ($\simeq$ 2.3 Å) as the Co layer thickness is increased. This scale parameter is insensitive to the thickness of the Py layers. In order to examine the relative importance of bulk scattering, EBS samples were prepared with atomically thin Co layers displaced into the interior of the Py layers. Magnetoresistance decreased rapidly with increasing displacement distance, on the same length scale, and saturated at the original value for Py/Cu. When Py interface layers were inserted in a Co/Cu EBS structure, GMR decreased with Py layer thickness on a length scale $\simeq$ 2.8 Å. A survey of other combinations of metals gave similar results in all cases studied, indicating the predominant effect of the magnetic/spacer interface on an atomic scale $\simeq$ 1.5 to 3 Å. A recent review of GMR experimental findings has been given by Parkin [12].

Fert and Bruno [13] and Levy [14] have recently reviewed experimental data and theory relevant to electrical conductivity in GMR materials. These authors discuss parametrized theoretical models that have been used to describe the enhanced magnetoresistance characteristic of these materials. The present paper concentrates on the theory of spin-dependent conductivity, developing a general formalism applicable to GMR materials. The physical basis of the observed enhanced magnetoresistance is discussed in Section 2. A general review of semiclassical and quantum transport theory is given in Section 3, while the question of nonlocal response is discussed in Section 4 in the context of Maxwell's equations for the local electric field. Parametrized semiclassical and quantum models of GMR are surveyed in Section 5. Section 6 surveys more recent theoretical studies based on *ab initio* energy-band calculations for the conduction electrons. General conclusions are summarized in the last section.

2. The physical basis of enhanced magnetoresistance

The essential physical process in GMR materials is spin-dependent dissipative scattering. One spin component of the electronic current is everywhere relatively weakly scattered if magnetization vectors in magnetized sheets or granules are aligned parallel to one another. In antiferromagnetic alignment, both spin components are equally strongly scattered. Experimental data and theoretical models indicate that the predominant spin-dependent scattering process is associated with the interfaces in layered elemental materials and with the grain boundaries in granular materials. This is consistent with data indicating a significant volume effect in permalloy, since an alloy might be considered to be a granular material with grains of atomic size throughout its volume. Although most experiments have been carried out in CIP geometry (conduction in-plane), the largest GMR ratios occur in CPP geometry (conduction perpendicular to the plane). This is consistent with a predominantly interfacial mechanism, since in CPP geometry the current must flow through all interfaces between the measuring leads, while in CIP geometry each conducting spacer layer acts as a current shunt.

As originally pointed out by Mott [15–17] and discussed in the textbook by Mott and Jones [18], the observed reduced conductivity of transition metals as compared to noble metals is due not to conduction by d-carriers but to transitions into empty d-states at the Fermi level in the transition metals. Because the s/p effective mass is much less than that of the d-electrons, s/p electrons are the principal charge carriers in both noble and transition metals. Any dissipative mechanism for scattering into unoccupied d-states at the Fermi level reduces the lifetime of conduction electrons. In a magnetized transition metal, this final-state effect causes the mean free path of minority electrons to differ from that of majority electrons. Hence, the conductivity depends on spin. In the two-fluid model it is an immediate consequence of Ohm's law that the two spin components of the conduction electrons, subject to different resistivities but sharing a common voltage drop, carry different current densities under steady-state conditions. This implies that the electronic current is spin-polarized, a result confirmed in detailed studies of the Boltzmann equation discussed below. A correct description of the spin-dependent Fermi surface is essential to any realistic theory of this Mott effect. If some scattering process is itself strongly spin-

selective, it provides a mechanism for spin-dependent conductivity in addition to the Mott mechanism. An important example is scattering by atoms interchanged randomly across the boundary of a magnetized layer or across the surface of a magnetized granule.

A magnetic material with spin-dependent conductivity must exhibit magnetoresistance, because within each magnetized layer or granule one spin component of the conduction electrons is subject to lower resistivity. A spin component can have this "correct" spin polarization sense throughout the material only if the local magnetization vectors are ferromagnetically aligned. If the alignment is antiferromagnetic or random, the electronic current must flow at least in part through regions or domains in which the magnetization direction differs, so that both spin components are subject to relatively strong scattering in some region. This implies enhanced resistivity. Magnetoresistance is always reduced by spin-flip scattering, since the distinction between the two spin polarizations is lost. In order for the spin sense to be retained between magnetized layers or granules, the intervening distance must be smaller than the mean free path for spin-flip (spin diffusion length). This is a necessary condition for validity of the two-fluid model and for GMR due to spin-dependent scattering. Values of the spin-dependent mean free path due to spin-conserving dissipative scattering, which determines the spin-dependent conductivity, are generally much shorter than the spin diffusion length.

3. Transport theory

A quantitative theory of electronic transport requires simultaneous solution of the coupled Maxwell and Schrödinger equations of nonrelativistic electrodynamics. This formidable task must be simplified in order to derive any useful results for GMR materials, somehow without distorting or overlooking important elements of the problem. These elements include the necessarily irregular spin-dependent Fermi surfaces in these heterogeneous materials, and scattering processes due to lattice vibrations, structural irregularities, interfaces, and displaced atoms. Spin-flip scattering by magnons may become important at higher temperatures. There are several simplifying aspects of the GMR problem that can be exploited in constructing a practical theory. In particular, the materials of primary interest are macroscopic samples, for which it is unlikely that quantum effects beyond the usual electronic structure theory of metals and alloys are relevant. The interior regions of layers or granules may be sufficiently large and homogeneous that they have the properties of bulk materials. The electric and magnetic fields are of moderate strength, so that it is consistent to work in the linear-response limit of theory. In these circumstances, a quantum Boltzmann equation is valid and has the same physical validity as the more fundamental quantum Kubo theory [19–21]. This quantum formalism originated in work by Greenwood [22], who showed that the semiclassical Boltzmann equation for impurity scattering could be derived in the limit of large relaxation time from the equation of motion for the quantum density matrix. Results of theory based on the semiclassical Boltzmann equation and on the Kubo formalism are expected to be indistinguishable if both describe the same physical system and scattering mechanisms at a comparable level of internal accuracy [23–25].

In order to incorporate the Mott effect into transport theory, an intermediate form of Boltzmann theory is used here. Identifying the eigenstates of self-consistent energy-band calculations with the electron quasiparticles of Fermi liquid theory, the Boltzmann theory is applied to the occupation numbers of these quasiparticles. This formalism has the advantage of maintaining conservation laws at each stage of computation, and of treating all scattering processes at a common level of theory. In this formalism, the distinction among physical properties of CIP, CPP, and granular GMR materials occurs at the level of solution of Maxwell's equations for macroscopic current flow, based on a common theory of microscopically averaged linear response or conductivity. It is postulated that the electronic states considered in the semiclassical Boltzmann theory of metallic conductivity [23] are the electron quasiparticles of Fermi liquid theory [26], computed with a Hamiltonian that includes electronic interactions but omits dissipative scattering processes. A scattering process is defined as "dissipative" here if it causes the energy of a quasiparticle to become complex. This distinguishes such processes as phonon scattering or scattering by random impurities from the phase-coherent scattering incorporated in the self-consistent construction of Bloch waves. The postulated electron quasiparticles are modeled by self-consistent energy-band calculations using the density-functional theory [27, 28], which includes electronic interactions and correlation. As eigenstates of the model system, these quasiparticles do not scatter from one another. A quasiparticle state is defined at each point on the spin-dependent Fermi surface. Considered as an application of the quantum Boltzmann equation [21], the theory developed here builds the real part of the interaction self-energy into the energies of Bloch waves. The imaginary part of the self-energy is attributed to dissipative scattering processes. Since the energy-band model omits dissipative scattering completely, except in the case of alloys, such processes must be treated by perturbation theory in the quasiparticle basis. Dissipative scattering rates are defined point-to-point over the Fermi surface as transition rates between quasiparticle states. This Boltzmann formalism in principle requires

computation of the net lifetime, subtracting the scattering-in rate from the decay rate at all points on the Fermi surface.

For a regular periodic solid or superlattice model system, noninteracting quasiparticles are indexed by a spin index s, by a band index b, and by momentum $\mathbf{k}$. Each quasiparticle state is modeled by a wave packet constructed from a Bloch wave with specified parameters $(s, b, \mathbf{k})$. When these parameters are denoted by a single index k, the energy of a quasiparticle is a real number ϵ_k, determined by the self-consistent density-functional model. In the presence of a local electric field $\mathscr{E}$, Ehrenfest's theorem determines mean time-derivatives of the momentum and position of an electron described by such a wave packet. The implied group velocity is $\mathbf{v}_k = (1/2\hbar)\nabla_{\mathbf{k}}\epsilon_k$, given ϵ_k in Rydberg units. The statistical distribution function for quasiparticles is the occupation number f_k. In linear-response theory, the steady-state occupation probability f_k is approximated by the Fermi–Dirac distribution function f_0 plus an incremental term $g_k = f_k - f_0$ that is proportional to the driving field. The mean value of electric current density for each quasiparticle is $\mathbf{j}_k = -e\mathbf{v}g_k$. A steady-state Boltzmann transport theory based on these postulates and definitions is developed here.

In a homogeneous material or superlattice with no thermal gradient, a Bloch wave defines the probability of finding an electron with specified parameters $(s, b, \mathbf{k})$ at a point $\mathbf{x}$. At the Fermi surface, the mean velocity of such an electron is the Fermi velocity $\mathbf{v}_k$. If there is a thermal gradient, f_0 must vary with position as the temperature parameter changes. In an inhomogeneous material, the response increment g_k must vary with position as the local conductivity changes. In the general case, $f_k(\mathbf{x})$ defines the local statistical occupation probability of a quasiparticle state modeled by the Bloch wave $\phi_k(\mathbf{x})$. In this interpretation of the Boltzmann theory, phase information is contained in the Bloch wave, but not in the distribution function f_k. Neglecting thermal gradients, f_0 is constant, while both g_k and $\mathscr{E}$ can be considered to vary on a length scale larger than a typical atomic radius, but smaller than the extent of a Bloch wave packet. If $\mathscr{E}$ varies within a polyatomic translational unit cell, the continuity equation for the current density requires g_k to vary on the same scale. This can be described in terms of nonlocal response or by local averaging for inhomogeneous materials. Such extensions of the theory are discussed in the following section.

In a steady state, the incremental occupation probability g_k for each quasiparticle is determined by balancing the rate of change at a fixed point $\mathbf{x}$ due to transport away from that point, and to conversion of the state $(s, b, \mathbf{k})$ into other states $(s', b', \mathbf{k}')$ by the driving field, against the net rate of change due to dissipative scattering. This is expressed in a quasiparticle Boltzmann equation indexed by $k = (s, b, \mathbf{k})$,

$$\mathbf{v}_{\mathbf{k}} \cdot \nabla g_k - \frac{e}{\hbar}\mathscr{E} \cdot \nabla_{\mathbf{k}} f_0 = \sum_{k'} (g_{k'} - g_k) P_{k',k} , \tag{1}$$

assuming symmetry of state-to-state transition probabilities P. Neglecting spin-flip transitions, the sum over index k' here denotes a sum over band index b' and an integral over the reduced Brillouin zone in k-space. This integral is weighted by the number-of-states element for each spin, $(\Omega/16\pi^3\hbar v)d\epsilon dS$, for energies in rydbergs. Here Ω is the volume of the translational unit cell and dS is the area element of an energy surface. The Mott final-state effect results from the dependence of this formula on electron velocity and on Fermi surface area. The electric field must be a local solution of Maxwell's equations. This implies nonuniformity in inhomogeneous materials, requiring consistent local averaging of g_k and $\mathscr{E}$.

The two scattering terms on the right-hand side of Equation (1) represent scattering-in and scattering-out, respectively. The scattering-out terms define a quasiparticle lifetime $\tau_{k,\text{out}}$ such that $\tau_{k,\text{out}}^{-1} = \Sigma_{k'} P_{k',k}$. To include scattering-in terms, it is convenient to define a net relaxation time $\tau(s, b, \mathbf{k})$ such that the right-hand side of Equation (1) takes the simple form $-\tau^{-1}g$. The defining equation is

$$\tau_k^{-1} g_k = \tau_{k,\text{out}}^{-1} g_k - \sum_{k'} P_{k,k'} g_{k'} , \tag{2}$$

again using the symmetry of state-to-state transition probabilities. Since g is a scalar function of the electric field vector, in linear response theory it must take the form $C\mathbf{\Lambda}_k \cdot \mathscr{E}$. This defines a vector mean free path $\mathbf{\Lambda}_k = \tau_k \mathbf{v}_k$ in terms of a net relaxation-time tensor τ_k. With these definitions, Equation (2) is equivalent to

$$\mathbf{\Lambda}_k = \tau_{k,\text{out}}\left(\mathbf{v}_k + \sum_{k'} P_{k,k'}\mathbf{\Lambda}_{k'}\right), \tag{3}$$

for iterative computation of the scattering-in terms [29, 30]. If there is a thermal gradient, or in an inhomogeneous material, the constant C becomes a function $C(\mathbf{x})$. In applying transport theory to substitutional alloys, random composition implies a dissipative scattering effect at the level of the self-consistent coherent potential approximation (CPA) [31]. So long as the resulting energy width is small at the Fermi level, real energies ϵ_k acquire an imaginary part $-(i/2)\gamma_k$ corresponding to a quasiparticle lifetime $\tau_{0,k} = \hbar/\gamma_k$. This implies an intrinsic time decay of the quasiparticle occupation numbers. Since Equation (1) is expressed here in the context of energy-band theory with real energy values, such an intrinsic lifetime could be parametrized by

adding a term of the form $\tau_0^{-1} g$ into the left-hand side of this equation and into the right-hand side of Equation (2). For consistency, scattering due to random occupation of lattice sites, treated by CPA, must then be omitted from the detailed mechanisms included in the transition probabilities $P_{k,k'}$.

Using the definitions of Fermi velocity and vector mean free path given above, the quasiparticle Boltzmann equation takes the form

$$\mathbf{\Lambda_k} \cdot \nabla g_k + g_k = 2e \frac{df_0}{d\epsilon_k} \mathbf{\Lambda_k} \cdot \mathscr{E}. \tag{4}$$

This is an inhomogeneous diffusion equation for each quasiparticle at the Fermi surface. The first term here (diffusion term) vanishes in the interior of a homogeneous solid if there is no thermal gradient. It must be included when considering effects near an external bounding surface, as in the semiclassical Fuchs–Sondheimer theory [32, 33]. The electric current density is the sum of terms $\mathbf{j} = -e\mathbf{v}g$ for all quasiparticle Bloch functions at the Fermi level. This sum is related to the mean local electric field by a conductivity tensor such that $j_i = \Sigma_j \sigma_{ij} \mathscr{E}_j$. The conductivity tensor is derived by weighting g_k from Equation (4) by the density of states and integrating over an energy range about the Fermi energy. If diffusion terms are neglected and the derivative of f_0 is replaced by an energy delta function, this gives

$$\sigma_{ij}(s) = \frac{e^2}{8\pi^3 \hbar} \sum_b \int_{\epsilon=\epsilon_f} n_i \Lambda_{k,j} \, dS, \tag{5}$$

where $\mathbf{n}$ is a unit vector normal to the Fermi surface. The conductivity tensor is an integral over the Fermi surface of the tensor $\mathbf{n}\mathbf{\Lambda}$. If the net relaxation time is a scalar quantity, this reduces to $\mathbf{n}\lambda_k\mathbf{n}$, where $\lambda_k = \tau_k v_k$, defined by values of τ_k and $\mathbf{v}_k$ evaluated at each point $(s, b, \mathbf{k})$.

The diffusion term in the Boltzmann equation describes the net effect of transport by convection due to the group velocities of quasiparticle wave packets. This can be neglected in the interior of a uniform metal if there is no thermal gradient, but there is an asymmetrical effect near an external boundary. Since all wave functions vanish outside such a boundary (neglecting field emission or tunneling into a classically forbidden region), transport to an internal point by convection from the exterior must vanish. This requires g_k to vanish on the external boundary if the velocity $\mathbf{v}_k$ is directed inward. If the driving field $\mathscr{E}$ is uniform, the value of g valid in the interior of a uniform metal is a particular solution of the Boltzmann equation. To satisfy the boundary condition, a solution of the homogeneous diffusion equation is subtracted which exactly cancels the particular solution at the boundary for each inward-directed group velocity. This subtracted term decreases exponentially into the interior with a length scale given by the projected mean free path $\mathbf{n} \cdot \mathbf{\Lambda}$, where $\mathbf{n}$ is the inward normal vector on the boundary surface. Thus, this boundary condition is propagated into the interior of a metal by the diffusion term in the quasiparticle Boltzmann equation, resulting in reduced conductivity.

The Fuchs–Sondheimer theory [32, 33] sums the g-functions considered here over all quasiparticles at the Fermi level and imposes this boundary condition. It is attributed to diffusive scattering at an external boundary. An additional parameter p is used to represent the relative probability of specular reflection, considered to be a physical process in competition with diffusive scattering. The discussion given above indicates that this is a false dichotomy. Diffusive scattering is not relevant to the truncation of wave functions due to an external potential barrier. Standing-wave functions with a fixed nodal surface establish a coherent phase relationship between two time-reversed traveling-wave components. Phase-coherent scattering processes due to static potential functions in the Schrödinger equation are fully taken into account in the construction of Bloch waves. Hence, they affect the Boltzmann equation only through properties of these wave functions, in the present case through vanishing electron number density outside a physical boundary surface. It is interesting to note that in several parametric studies of experimental data on thin films and wires, summarized by Sondheimer [33], the best value of the "specular reflection" coefficient p was found to be $p = 0$.

The most important consequence of the Fuchs–Sondheimer theory is that resistivity increases when geometrical dimensions are reduced to the scale of the mean free path in a metal. Large effects are observed for current flow parallel to a boundary surface [33]. This might appear to be counterintuitive, but it is important to recognize that electronic wave functions are not confined to a single atomic layer or to a precisely defined propagation direction. A useful conceptual model is that even in the absence of an external driving field, a very large number of electrons are moving in all directions in a normal metal, at very high velocity (the Fermi velocity). This dynamic swarm does not transport electric current, because the statistical net flow cancels exactly. An applied electric field produces a relatively small imbalance biased in the direction of the field, but the electron swarm still samples the entire material within the statistical mean free path. In this model, it is clear that any reduction of the mean free path must affect all components of the conductivity tensor, so that the large observed CIP effect is not inconsistent with confinement in the direction normal to the plane of net current flow.

For any regular periodic solid metal described as a Fermi liquid, the quasiparticle Boltzmann theory is

expected to be quantitatively correct if the underlying energy-band calculations are adequate. For metallic substitutional alloys, calculations and theoretical analysis by Butler and Stocks [31, 34] show that the Kubo formalism, without vertex corrections, and the Boltzmann formalism, without scattering-in terms, are at a common level of accuracy. Because a Green's-function formalism is used in the alloy theory, extension to the Kubo theory is quite natural, but the calculation of vertex corrections [24] appears to be very difficult to implement. Scattering-in terms can be included in the Boltzmann equation by solving inhomogeneous linear equations of large dimension [31], for which an iterative method is available [29, 30]. The fact that scattering-out and scattering-in terms are computed from the same set of state-to-state transition probabilities gives the Boltzmann theory the practical advantage that detailed balance is maintained within the formalism, avoiding artifacts such as spurious accumulation of occupation probabilities that are inconsistent with the basic steady-state condition. In the Kubo formalism [24, 35], scattering-out rates correspond to lifetimes deduced from self-energies, while scattering-in rates must be computed as vertex corrections.

4. Nonlocality and Maxwell's equations

Equation (1), the quasiparticle Boltzmann equation, is expected to be valid for any crystalline metal if the local electric field is averaged over the translational cell. If a homogeneous layer or granule of this metal is embedded in a macroscopically inhomogeneous material, the bulk conductivity should be valid for the interior of the layer or granule, but special consideration of the boundary region is needed. In the case of a cleaved surface of an otherwise regular periodic solid, all properties of electronic wave functions remain valid in the interior, but the wave functions must terminate at the boundary. This is modeled in the Boltzmann equation by allowing the incremental distribution function g to vary in space in the boundary region, while retaining the energy and Fermi velocity of each Bloch function as in the uncut solid. In CIP geometry, the local electric field is constant and the current density is proportional to the g-function. In CPP geometry, the current density is constant and the local electric field must vary inversely with the g-function. In either case, conductivity is reduced in the boundary region, as derived in the Fuchs–Sondheimer theory. This example shows that g and the electric field must be treated consistently in boundary or interface regions. Attributing spatial variation to g does not imply that wave functions can be localized on the same scale. For example, the truncated Bloch waves in a semi-infinite solid are still delocalized over its full volume. It is consistent with the linear-response model to represent a response varying on the length scale of the mean free path in a basis of unperturbed wave functions that are uniform in a larger region, using coefficients or weight functions that vary on the lesser of the two length scales. Different theoretical models, discussed below, consider wave functions defined globally for a layered material or only locally for a subset of layers. A global definition may require a density-matrix formalism for an inhomogeneous material or when the elastic mean free path is small compared with relevant geometrical structures, such as layer spacings, because the phase coherence implied by well-defined wave functions is lost.

The nonlocal conductivity tensor is defined in the fully coupled linear-response theory as the kernel of a linear integral operator,

$$\mathbf{j}(\mathbf{x}) = \int \sigma(\mathbf{x}, \mathbf{x}')\mathscr{E}(\mathbf{x}')d^3\mathbf{x}', \tag{6}$$

where $\mathbf{j}$ is the current density and $\mathscr{E}$ is the local field derived by solving Maxwell's equations as determined by the conductivity tensor. If magnetization vectors are collinear and if spin-flip scattering can be neglected, each spin component of $\mathbf{j}$ satisfies a similar equation. Because the electric field cannot carry an electronic spin index, this defines a separate conductivity tensor for each spin component of $\mathbf{j}$.

The electric field relevant to conductivity is an infinitesimal perturbation of the Coulomb field in the density-functional Schrödinger equation. Averaging either this electric field or the current density over an atomic cell is assumed here to be a valid approximation, as it should be except for very large current density or very strong fields. If the local field varies sufficiently slowly on an atomic scale, only the average of the conductivity tensor over each atomic cell affects the Maxwell equations for steady-state current flow in a heterogeneous macroscopic material. Averaging over each atomic cell, and approximating the electric field within each cell by its mean value in that cell, Equation (6) for the cell indexed by μ reduces to a linear algebraic expression,

$$\mathbf{j}_\mu = \sum_\nu \sigma_{\mu\nu}\mathscr{E}_\nu, \tag{7}$$

summed over cells indexed by ν. It should generally be valid for GMR materials to approximate the nonlocal (two-point) conductivity tensor by the response matrix defined in Equation (7), indexed by atomic cells. This provides a finite-element representation of the classical Maxwell equations for steady-state current flow. They could be solved by summing partial solutions obtained in a diagonalized representation of the response matrix.

For a regular periodic solid or superlattice model of a layered or inhomogeneous material, the conductivity response matrix defined in Equation (7) can be restricted

to indices for atomic cells within a single translational cell, by summing over all translationally equivalent atoms. Following Zhang and Butler [36], the linear Boltzmann equation can easily be adapted to compute the incremental distribution function as a matrix with the same structure as the conductivity matrix, indexed by atoms in a translational cell. This is done for the quasiparticle Boltzmann equation by computing g_k separately for constant electric field elements, one for each atomic cell and for each coordinate axis, and then constructing linear combinations of the response elements such that the equations of continuity for current density and electric field are satisfied to the extent consistent with averaging over atomic cells. This construction requires only the subdivision of quasiparticle or Bloch wave occupation numbers into partial atomic occupation probabilities, which are always computed in a self-consistent energy-band calculation.

If the electric field varies sufficiently slowly that it can be replaced by an average, denoted by $\mathscr{E}^{\mu}$, over atomic cells in a neighborhood of a particular cell μ, and if the nonlocal conductivity tensor $\sigma_{\mu\nu}$ vanishes sufficiently rapidly as the distance between atomic cells ν and μ increases, the averaged value of $\mathscr{E}$ can be substituted into Equation (7), which reduces to the form

$$\mathbf{j}^{\mu} = \sigma^{\mu} \mathscr{E}^{\mu}, \tag{8}$$

where

$$\sigma^{\mu} = \sum_{\nu} \sigma_{\mu\nu}. \tag{9}$$

These assumptions are inherent in applications of the usual semiclassical Boltzmann equation to regular periodic solids. They define a local response model (LRM). When this model is valid in some region of an inhomogeneous system, the solution of Maxwell's equations simplifies in this region to solution of a classical potential problem, since a constant local conductivity tensor is associated with each atomic cell. The local electric field is computed by solving a (tensorial) Laplace equation for the scalar potential. At a cell boundary, the normal component of the current density and the tangential component of the electric field must be continuous. The equation of continuity holds rigorously for the current density.

The local response model provides a rationale for applying the quasiparticle Boltzmann equation to inhomogeneous macroscopic materials. The basic idea is to use the best possible representation of the near environment of each atomic cell to compute a set of Bloch wave functions at the Fermi level, obtained by a self-consistent supercell or layer KKR [37] calculation. These wave functions are not localized, but they are associated with an atomic cell. The construction outlined above, computing the linear response to atomic components of the electric field, then combining these linear elements to satisfy the continuity conditions required by Maxwell's equations, gives a conductivity response matrix indexed by atoms within a translational unit cell. Tensorial elements of this matrix are determined by any three linearly independent electric field solutions. Designating a particular atomic cell by index μ, the quasiparticle Boltzmann equation for each of these electric field solutions defines an incremental distribution function g_k^{μ}, for quasiparticles indexed by k. With all quantities averaged over atomic cells, the conductivity response is

$$\mathbf{j}^{\mu} = -e \sum_{k} \mathbf{v}_k g_k^{\mu}. \tag{10}$$

In this construction, the electric field elements $\mathscr{E}_{\nu}$ must vary in proportion to the particular element $\mathscr{E}_{\mu}$ when each electric field solution is multiplied by a constant. This implies that the atomically averaged field elements are related by constant tensorial coefficients. Summing these coefficients over the translational cell gives an effective single-atom local response corresponding to the LRM. Thus, the LRM model can be assumed as an Ansatz when calculations are subdivided into linear elements that are combined to give a total g-function and electric field consistent with Maxwell's equations, in the step-function approximation implied by averaging all quantities over atomic cells. This construction can be rationalized by noting that it is physically impossible to produce a local electric field that does not satisfy Maxwell's equations. A formalism that is valid only for such solutions is in fact completely general for physical systems.

The usual Boltzmann formalism for the conductivity tensor of a model superlattice assumes uniform electric field in the translational cell, which is not generally valid for polyatomic cells. The modification proposed here for inhomogeneous magnetic materials is to associate a spin-dependent conductivity tensor with each atomic cell, appropriate to its near environment in the actual material under study. Spatial variation of conductivity near an external boundary should be computed as in the Fuchs–Sondheimer theory. In general, the local electric field must be computed by combining partial solutions of the Boltzmann equation so that the sum is consistent with Maxwell's equations, although this may not be necessary in simple geometries. If tetragonal symmetry is assumed for layered systems, the principal axes of local conductivity tensors are the same in all layers. Thus, CIP and CPP geometries are separately described by local conductivity tensors whose elements have different numerical values. In CIP geometry, the in-plane electric field is constant in each uniform layer and must be continuous across layer boundaries. Hence, the local field is uniform throughout a layered material, and the current density varies from layer to layer in proportion to the local in-plane conductivity. In

CPP geometry, the current density normal to the layers must be uniform and continuous, while the electric field varies inversely to the local normal conductivity.

5. Parametrized models

In the Fuchs–Sondheimer theory [32, 33] of thin-film conductivity, geometrical confinement of conduction electrons is described by a boundary condition on the electronic distribution function. The incremental function g must vanish at an external boundary for velocities directed inward from the boundary. The influence of this boundary condition is propagated into the interior of a conductor by the diffusion term in the Boltzmann equation. This effect on g occurs in a surface layer whose thickness is measured by the mean free path of the electrons, which is several hundred angstroms in normal metals at laboratory temperatures. It explains an experimentally observed increase in resistivity for geometrical confinement of electrons on a length scale comparable to or less than their unconstrained mean free path. Camley and Barnaś [38] extended this theory to magnetic multilayers. The parametric model of Camley and Barnaś has been used extensively to study GMR materials. A spin-dependent incremental electronic distribution function $g(v_z, z)$ is assumed to be a function only of the coordinate z orthogonal to the planes of a layered material and of the component v_z of the Fermi velocity. The local electric field $\mathscr{E}$ is assumed to be a constant vector in the tangential direction x. The simplified Boltzmann equation used in this model is

$$\tau v_z \frac{\partial g}{\partial z} + g = \frac{e\tau\mathscr{E}}{m}\frac{\partial f_0}{\partial v_x}, \tag{11}$$

where f_0 is the Fermi–Dirac function. In nonplanar geometry the first term becomes $\mathbf{\Lambda} \cdot \nabla g$ [39]. Equation (11) is of the same form as the quasiparticle Boltzmann equation (4) except that the distribution functions are summed over all quasiparticles at the Fermi level. Spin-dependent relaxation times are associated with the interior of each layer. The relaxation-time parameters in this model can be considered to be averages of quasiparticle lifetimes whose detailed values would exhibit the band-structure effects considered by Mott. Empirical values of these parameters do not distinguish among different microscopic scattering mechanisms.

Since the incremental distribution function g in Equation (11) varies with coordinate z, the model requires specifying the relationship between values of g across internal boundaries. The rotation of spin quantization axes between magnetized layers is modeled by spin-dependent transmission coefficients. Spin-dependent diffusive scattering parameters are assigned to each internal interface [38]. The physical basis for the Fuchs–Sondheimer boundary condition has been discussed above in connection with the quasiparticle Boltzmann theory. For reasons given there, it is not obvious that variation of g, considered as a distribution of occupation numbers for Bloch wave functions that are continuous over many atomic layers, can be defined by boundary conditions at interfaces on the atomic scale. In particular, introduction of specular reflection coefficients at layer boundaries may not be justified. In fact, the reflection coefficients have been set to zero in applications of the Camley and Barnaś theory. It was found to be difficult to fit the strong interface scattering observed experimentally with the spin-dependent diffusive scattering parameters of the original theory. Much better agreement was obtained when interface scattering was treated as spin-dependent bulk scattering in a thin interface mixing layer [40, 41]. Inoue and Maekawa [42] modeled the expected strong spin-dependent scattering effect of randomly displaced magnetized interface atoms in terms of random exchange potentials.

The ratio of diffusive scattering parameters $D_\downarrow/D_\uparrow$ describes the effect of spin-selective dissipative scattering at an interface. As noted by Baibich et al. [1] in presenting their original GMR experimental data, this ratio can be approximated by the experimental ratio $\alpha = \rho_\downarrow/\rho_\uparrow$ of the incremental resistivities due to isolated impurities in a magnetized host metal [43]. Camley and Barnaś [38] used the experimental value of α for Cr impurities in bulk Fe in their model calculations. If atoms of the spacer and magnetic metal were exchanged randomly across an interface, the resulting spin-dependent impurity scattering would be proportional to this ratio, and to the concentration of such displaced atoms in the vicinity of the interface. Distortion described as interface roughness on a macroscopic scale requires detailed modeling if the length scale of the roughness is comparable to the experimentally very short mean free path associated with interface scattering. Geometrical irregularities on a larger scale could not affect an essentially atomic scattering mechanism. Together with layer thicknesses, the important parameters of the simplified Boltzmann equation (11) are bulk mean free paths and the experimental ratio α. Fert and Bruno [13] show that these parameters can be used directly in a classical circuit model of the magnetoresistance, which depends only on α in the limit of infinite bulk mean free path. A similar resistor network model has been used by Mathon and collaborators [44–46].

GMR increases with decreasing temperature because spin-mixing due to magnon scattering decreases and because spin-independent bulk scattering by various mechanisms (structural irregularities, phonons) decreases. The model of Camley and Barnaś [38] omits effects of magnon scattering and cannot distinguish spin-dependent

energy-band effects (the Mott effect) from spin-selective impurity scattering. Using the same bulk mean free path λ for Cr and Fe in Cr/Fe, values of λ required to fit the temperature variation of GMR increased from 180 Å to 6000 Å over the range from room temperature down to 4.2 K [38]. This low-temperature value of λ is unrealistically large. An analytic solution of the simplified Boltzmann equation was derived and applied to study the relationship between mean free path and the magnetoresistance ratio [47], modeling spin-dependent scattering only at interfaces. Values of the mean free path at low temperatures were found to be in reasonable agreement with experimental values. Applications of the model of Camley and Barnaś include a study of Fe/Cr and Co/Au multilayers [48], and a study of spin-dependent bulk scattering in permalloy-based spin-valve structures [49].

Valet and Fert [50, 51] used the Camley and Barnaś model to consider CPP geometry. Assuming uniform current flow, the Boltzmann equation determines the electric field or scalar potential function consistent with steady-state conditions. A spin-dependent chemical potential is added to the scalar potential to account for spin accumulation if that should occur. When the spin diffusion length is large compared with the mean free path, the simplified Boltzmann equation reduces to a macroscopic model in which the parameters are spin-dependent mean free paths and chemical potentials. Assuming a spherical Fermi surface not indexed by spin (constant magnitude of the Fermi velocity), conductivity is proportional to mean free path with the same factor for both spin directions, and the spin-dependent current density is proportional to the product of conductivity and local electric field. This derivation justifies a formula that equates a simple function of measured resistivities to a linear function of the number of bilayers in a multilayer material of fixed total thickness. The coefficients in this linear formula determine the bulk spin asymmetry coefficient β and the interfacial spin asymmetry coefficient γ, which can thus be deduced from experimental data [52–54]. If the chemical potential parameters vanish, the macroscopic equations simply state Ohm's law separately for the two spin components of the current density. The local electric field derived from Maxwell's equations is not indexed by spin. Valet and Fert [50, 51] consider only collinear magnetization. If the magnetization in successive magnetic layers is not collinear, the quantization axis for electronic spin must be rotated, which may cause spin-flip scattering in analogy to magnetic domain theory. This subject is beyond the scope of the present review.

Levy and Zhang [14, 55] have recently reviewed parametric models of GMR based on quantum theory. The theory was derived for layered materials by Levy et al. [56, 57], by Vedyayev et al. [58], and with some revisions by Camblong et al. [59–62]. Kubo formalism is used rather than the Boltzmann equation. Green's functions are computed using a free-electron Hamiltonian with delta function scattering potentials whose spin-dependent coefficient parameters vary from layer to layer, including both bulk and surface terms. Because a free-electron model is used, spin-dependent Fermi surface and Mott effects are not included directly. The essential parameters are the spin asymmetry parameter α, which may be different for bulk and surface scattering, and the layer thickness.

In the Kubo linear-response theory [24, 35], the two-point conductivity tensor is a current–current correlation function, expressed in terms of the Green's function for an exact solution of the N-electron Schrödinger equation, including all potential functions or operators responsible for dissipative scattering. Since dissipative scattering is a statistical process, as in the case of random impurities, some statistical assumption is already inherent in the definition of this Green's function. This is explicit in applications to substitutional alloys, using the CPA (coherent potential approximation) model [31]. Camblong [60] develops the Kubo formalism in real space, for inhomogeneous conductors. In-plane periodicity is assumed. The formalism uses a mixed representation defined by in-plane momentum and normal coordinate z. If spin-flip transitions are neglected and magnetization is collinear, then

$$\sigma_\alpha(\mathbf{r}, \mathbf{r}') = \frac{4}{\pi}\frac{e^2}{\hbar}\left(\frac{\hbar^2}{2m}\right)^2 A_\alpha(\mathbf{r}, \mathbf{r}')\overleftrightarrow{\nabla}_{\mathbf{r}}\overleftrightarrow{\nabla}_{\mathbf{r}'}A_\alpha(\mathbf{r}', \mathbf{r}), \tag{12}$$

where α is a spin index. Here

$$\overleftrightarrow{\nabla}_{\mathbf{r}} = \overrightarrow{\nabla}_{\mathbf{r}} - \overleftarrow{\nabla}_{\mathbf{r}}, \tag{13}$$

where the arrows indicate an operator acting to the right or left, respectively, and

$$A_\alpha(\mathbf{r}, \mathbf{r}') = -\operatorname{Im} G^{\mathrm{ret}}_{\alpha\alpha}(\mathbf{r}, \mathbf{r}'), \tag{14}$$

in terms of the retarded Green's function. Assuming in-plane uniformity of multilayers, which implies a statistical average of dissipative scattering built into the Green's function and also that the local electric field is uniform in each plane, the nonlocal conductivity tensor can be integrated in each plane to give a two-point tensor in the z coordinates only. This is

$$\sigma_\alpha(z, z') = \frac{4}{\pi}\frac{e^2}{\hbar}\int \frac{d^2k_\parallel}{(2\pi)^2}\left(\frac{1}{2}k_\parallel^2\mathbf{I}_\parallel + \bar{k}^2\mathbf{e}_z\mathbf{e}_z\right)[A_\alpha(\mathbf{k}_\parallel; z, z')]^2, \tag{15}$$

where $A_\alpha(\mathbf{k}_\parallel; z, z')$ is the in-plane Fourier transform of Equation (14). The integral here can be carried out analytically and expressed in terms of the functions

$$\phi_\alpha(z, z') = \int_{z_<}^{z_>} \frac{d\zeta}{\lambda_\alpha(\zeta)}, \tag{16}$$

in which $z_<$ and $z_>$ are the lesser and greater of z, z', respectively; λ_α is an in-plane averaged spin-dependent mean free path. The principal elements of the conductivity tensor are

$$\sigma_\alpha^{\parallel}(z, z') = \frac{3C_D}{4}\{E_1[\phi_\alpha(z, z')] - E_3[\phi_\alpha(z, z')]\},$$

$$\sigma_\alpha^{\perp}(z, z') = \frac{3C_D}{2} E_3[\phi_\alpha(z, z')], \tag{17}$$

where $E_n(x) = \int_1^\infty e^{-tx} t^{-n}\, dt$ and $C_D = e^2 k_F^2/6\pi^2\hbar$.

The parametrized quantum theory has clarified some questions regarding the meaning of parameters introduced in the Camley and Barnaś model. In particular, it supports the use of angle-dependent transmission coefficients to represent the effect of spin-dependent scattering associated with interfaces [60]. The underlying physical model for interfaces is an atomically thin transition layer, interposed between two homogeneous metallic layers, in which very strong spin-dependent scattering can be treated as a volume effect. Introduction of this model [40, 41, 56, 63, 64] significantly improved the parametric fit to experimental data that showed strong interface scattering. Because the Green's-function formalism derives a nonlocal response function, valid for any assumed local electric field, it can treat both CIP and CPP geometries, as well as granular materials, with the same theoretical model. As pointed out above, the electric field must vary inversely to the local conductivity in CPP geometry. A very important general result obtained with the parametrized quantum theory [14, 61, 65, 66] is that for the same scattering model, CPP magnetoresistance will always be greater than CIP magnetoresistance, possibly by a large factor. This follows from the fact that magnetoresistance depends on the spin-dependent dissipative scattering integrated along a current path. CIP magnetoresistance is always reduced by current shunting through the spacer layer, going to zero when the spacer layer thickness becomes greater than the mean free path in the spacer metal. CPP magnetoresistance depends on the global pattern of magnetization, not on the internal arrangement of magnetic layers [65]. This supports a simple classical resistance model that has been very useful in interpreting CPP experimental data [54, 65, 67]. The theory indicates that properties of granular materials and layered materials in CPP geometry should be similar [67, 68], and has been used to study granular Cu–Co alloys. Spin-dependent scattering is attributed to surface boundaries of Co particles and to bulk scattering in the interior of these particles [69].

The quantum model has in general confirmed conclusions of the semiclassical Boltzmann model, but both have similar limitations. The implications of Mott's analysis of electronic conduction in transition metals cannot be examined in terms of the simple spin-independent spherical Fermi surfaces used in these models. While the Kubo formalism is in principle more fundamental, its full implementation involves such formal and practical difficulties that essential aspects of physical processes may be omitted or overlooked. Formalism based on a nonlocal conductivity response does not appear to be required in treating either the CIP or CPP geometry, as shown in the simplified Boltzmann model of Valet and Fert [50, 51] for CPP geometry. Zhang and Butler [36] present a critical evaluation of the parametric models discussed here. These authors evaluate CIP and CPP layer conductivities exactly, using the Kubo formula, for the quantum model of free electrons and random point scatterers (FERPS). In the semiclassical limit, the exact Kubo formula gives Equations (17), in agreement with Camblong and Levy [59, 60]. Calculations using exact theory in this limit agree well with the parametrized Boltzmann equation, but differ from the approximate quantum theory of Levy et al. [56, 57] when the mean free path is comparable to layer thicknesses. Exact Kubo calculations in the FERPS model, carried out by Zhang and Butler [70] for FeCr multilayers, confirm the general conclusion that an important cause of enhanced magnetoresistance is dissipative scattering due to interdiffusion of atoms across interfaces.

The Fuchs–Sondheimer theory may have nonphysical consequences for microscopically thin films [71]. In particular, a diffusely reflective boundary would induce no resistivity in the absence of impurity scattering. A modified theory [71], valid in the limit of vanishing bulk scattering, obtains nonzero resistivity due to surface roughness as a quantum effect. This theory agrees better with experimental data on thin films with a very long mean free path [72] than does Fuchs–Sondheimer theory, even assuming large values of the specularity parameter. Zhang and Butler [36] have recently evaluated thin-film conductivity in the FERPS model, comparing the exact Kubo formula with Fuchs–Sondheimer theory. Existing experimental data can be fitted by correcting semiclassical theory for zero-point motion of the electrons perpendicular to the film plane and by allowing the mean free path to depend on the direction of the Fermi velocity.

Although quantum effects are probably not important for typical macroscopic GMR materials, ballistic transport theory has been invoked in several theoretical models. In the extreme limits of high material purity (very long mean free path) and small geometrical dimensions, a metallic conductor acts as a quantum wave guide for electrons. The electronic wave functions, determined by boundary

conditions, provide a discrete number of transmission channels through the wave-guide region. If dissipative scattering in the wave guide is negligible, the conductance given by the Landauer–Büttiker formula [73, 74] is the quantized expression $(e^2/h)N$, where N is the number of transmission channels. In this ballistic limit, dissipation of energy takes place only in the contact region. Bauer [75] uses the Landauer–Büttiker formula including internal scattering to study CPP transport. The conductance G is the sum over all transmission channels,

$$G = \frac{e^2}{h} \sum_{nm,s} |t_{nm,s}|^2, \tag{18}$$

where $t_{nm,s}$ is the scattering amplitude between transmission modes indexed by n and m, with spin s, neglecting spin-flip scattering. Spin-indexed square-well potential functions were used by Bauer to model Fermi surface and Mott effects, together with impurity concentration and potential parameters. A formula is derived that agrees with Zhang and Levy [65] when the square-well potentials vanish.

In its original form, the Fuchs–Sondheimer theory models and explains the increased resistivity of thin strips or films due to geometrical confinement. As applied by Camley and Barnaś, this was extended to include parametrized diffuse scattering at interfaces in layered structures and spin-dependent transmission coefficients. Examined in detail, the most important source of the observed GMR appears to be spin-selective dissipative scattering in or near the interfaces between magnetic and spacer layers, or at the boundaries of granules. In the two-fluid model, the strong interface scattering is essentially transparent to one of the spin fluids, which is not affected by this scattering when layer magnetizations are parallel. For antiparallel or randomly oriented layer magnetizations, mean free paths are reduced equally for both spin fluids, and the total conductivity is reduced. Since this happens for layered systems of considerable thickness, the electronic wave functions are well approximated by assuming semi-infinite geometry, and are not confined to individual material layers. In view of this, the Fuchs–Sondheimer confinement effect is probably not directly involved in the observed large magnetoresistance, although it must be taken into account with respect to the outer boundary (vacuum interface). For a strip of given thickness, the confinement effect produces the greatest reduction of conductivity for the largest value of mean free path [33]. In the two-fluid model, this occurs for the favored spin component. It follows that the confinement effect actually reduces the magnitude of the GMR ratio, whose large observed values must arise from some more specific mechanism.

The mean free path in Equation (5) is a product of two factors, a relaxation time τ and the Fermi velocity v, which may be determined by very different aspects of the underlying physics. A parametrized spin-dependent mean free path may not help to distinguish between alternative microscopic mechanisms. The Fermi velocity is a property of the spin-dependent Fermi surface for the particular material under consideration, while the relaxation time is characteristic of dissipative scattering effects that may be unrelated to the electronic structure of this material. Equation (5) implies that conductivity is dominated by the largest values of the mean free path. Thus, in examining the cause of enhanced magnetoresistance in particular materials, theory must consider the largest possible values of the Fermi velocity, hence the s/p conduction electrons in transition metals, and mechanisms for spin-selective reduction of relaxation time, hence strong scattering by any dissipative process. Since s/p energy bands are the least sensitive to local magnetization, any large spin-dependent effect must be due to a significant influence of magnetization on some strong scattering mechanism. To examine this issue requires a detailed theoretical treatment of spin-dependent scattering. This has been done in the *ab initio* calculations discussed below.

6. Models using *ab initio* band structure

Several groups have developed methodology capable of combining self-consistent energy-band calculations with transport theory. Butler et al. [76] use the layer KKR (LKKR) method [37] for self-consistent local density functional calculations of the electronic structure of layered materials. Because the LKKR method constructs electronic Green's functions directly, it is compatible with the Kubo formalism, and also with the coherent potential approximation (CPA) for substitutional alloys. This has made it possible to study permalloy spin-valve structures. Mertig et al. [77, 78] combine self-consistent superlattice calculations on layered magnetic materials with a Green's-function method for magnetic impurity scattering. Electrical conductivity is computed using the quasiparticle Boltzmann equation. Nesbet [79] combines self-consistent superlattice calculations, by the LACO full-potential method [80, 81], with perturbation-theory calculations of spin-dependent scattering from displaced atoms at interfaces, and uses the quasiparticle Boltzmann equation to compute spin-dependent conductivity. Schep et al. [82, 83] carry out self-consistent superlattice calculations, but then use this band structure only for calculations in ballistic transport theory, which is not appropriate to current CIP and CPP experiments with normal metals and magnetic alloys. Coehoorn [84, 85] uses self-consistent superlattice calculations to discuss induced moments at interfaces. Ni moments are reduced by contact with Cu at an interface, but stabilized by a Co monolayer. Atomic

moments are found to depend strongly on nearest-neighbor environment at an Fe/V interface, but to be insensitive to environment for Fe/Cr.

The LKKR method used by Butler et al. [76] explicitly constructs an electronic Green's function, but in order to facilitate computations, the electronic mean free path at the Fermi surface is parametrized and used in the quasiparticle Boltzmann equation, without scattering-in corrections. Calculations were done in CPP geometry only. CoCu superlattices were studied with up to six alternating layers of each metal [76]. Interdiffusion of the two atomic species at a concentration of 1% was treated by CPA alloy theory. In the absence of any other dissipative scattering mechanism, large values were computed for the magnetoresistance ratio, varying from factors of 9.80 to 21.23 depending on the number of atomic layers. Similar calculations on permalloy ($Ni_{80}Fe_{20}$) (denoted here by Py), in PyCu superlattices, obtained extremely large magnetoresistance ratios, varying from factors of 204 to 1633 depending on the number of layers. These very large ratios result from nearly zero resistivity computed for bulk permalloy in the absence of the dissipative scattering mechanisms present in the physical material but not modeled, and also from the neglect of spin mixing in the alloy. Recent *ab initio* CPA calculations by Banhart and Ebert [86] on NiFe alloys included the spin-orbit interaction and obtained residual resistivities and anisotropic magnetoresistance of the same magnitude as observed data at low temperatures.

Systematic calculations of layer-dependent nonlocal conductivity were carried out for trilayer Co/Cu/Co spin-valve structures [87, 88], using Kubo theory without vertex corrections. The physical model is that of Cu layers of varying thickness embedded in Co. The layers have (111) orientation in an fcc lattice. Quasiparticle lifetimes were parametrized, not computed from a first-principles model. In this study, the methodology was verified by computing the layer-dependent conductivity of a free-electron gas, subject to a specified bulk relaxation time, and by comparing results with the analytical model of Zhang and Butler [36]. Similar tests of both CIP and CPP conductivity were made for pure Cu and for both spin components of the current density of pure Co.

It has been known for some time that the energy-band structure of Cu at the Fermi level is very similar to that of the majority-spin bands in magnetized Co, but different from the minority-spin bands. This implies qualitatively that spin-up (majority) conduction electrons move freely between the two metals, while spin-down electrons are impeded by a potential mismatch. How this affects conductivity, which depends on dissipative scattering, has been discussed by Nesbet [79], who computed the implied strong spin-selective scattering due to interdiffusion of atoms across a layer interface. Butler et al. [87, 88] compute several quantities that are related to this mismatch at interface boundaries. The number of majority-spin electrons per atom in the layered structures is very similar for Cu and Co, 5.5 and 5.35, respectively, while the number of minority-spin electrons on Co is only 3.65. The density of states at the Fermi level is very similar for majority electrons in Cu and Co but is much larger for minority electrons in Co, as are the d-wave phase shifts for the phase-coherent potential scattering that determines energy-band structure. These data are consistent with strong spin-dependent (or spin-selective) dissipative scattering by atoms displaced at an interface. Calculations in which a parametrized value of the quasiparticle lifetime was set equal for all states at the Fermi level gave very small magnetoresistance. A more detailed model used different relaxation-time parameters for Cu and Co, the same for both spins. The values used were appropriate to room-temperature bulk resistivities of 2.8 $\mu\Omega$-cm for Cu and 14.8 $\mu\Omega$-cm for Co. The scattering rate for majority-spin Co at the interface was set equal to twice the bulk value and, for minority electrons, to 24 times the bulk rate. These numbers were taken from CPA alloy calculations for Cu impurities in Co and for spin-aligned Co impurities in Cu. Layer-dependent conductivities computed with these parameters show large magnetoresistance.

In a third series of calculations, the Mott final-state effect was modeled by assuming that the electron lifetime for majority carriers in the Co bulk layers is seven times the corresponding rate for minority carriers. With lifetime parameters assigned separately to Cu and Co, spin-up and spin-down, and to bulk vs. interface layers, the layer-dependent conductivity was computed and showed large magnetoresistance. These calculations reinforce the conclusion that spin-dependent scattering from atoms displaced across an interface is an important mechanism for enhanced magnetoresistance, and they add new information on purely band-structure effects. Similar calculations were carried out by Nicholson et al. [89] to study the reduction of magnetoresistance due to nonferromagnetic atoms at Ni/Cu and Py/Cu interfaces in spin-valve structures. The Ni atomic moment is found to be reduced by contact with Cu. At Py/Cu interfaces, the Fe moments become disordered due to weakening of the effective interatomic exchange interaction. Butler et al. [90] give details of the theory relevant to alloys. Results of these studies have been summarized and discussed by Butler et al. [91]. This summary includes a survey of spin-dependent matching of effective potential functions in the transition metals, and indicates that the close match of spin-up potentials in layered CoCu has counterparts in PyCu, with a three-way match among Ni, Fe, and Cu, and in FeCr, favoring spin-down electrons in the latter case. Studies by this group show quite large ratios between

majority and minority carrier conductivities in NiFe and NiCo alloys.

Strong spin asymmetry of scattering by impurities in transition-metal matrices is well established experimentally and has been considered to be a likely cause of enhanced magnetoresistance since the first observations of GMR [1]. Quantitative theoretical studies of residual resistivity have been carried out by Mertig et al. [92–94] on Ni and ternary alloys. The method used, described in detail by Zeller [95] and applied to dilute Co alloys by Stepanyuk et al. [96], is an application of multiple-scattering theory using the muffin-tin model and local-density approximation (LDA) in a Green's-function formalism. Spin-dependent charge densities, taken from self-consistent calculations on the elemental metals, are used to construct the structural Green's-function matrix for the host crystal. Each muffin-tin sphere is characterized by a scattering t-matrix, so that an isolated substitutional impurity defines an incremental matrix Δt at the site of substitution. The Green's function for the perturbed system is related to that of the host crystal and to Δt by a matrix Dyson equation. The local scattering matrix Δt is transformed into a nonlocal matrix T that incorporates multiple scattering effects, using another algebraic equation that involves the structural Green's function [93]. Point-to-point transition probabilities over the Fermi surface are computed from the T-matrix and used in the quasiparticle Boltzmann equation to compute the residual resistivity proportional to the concentration of impurity atoms. Scattering-in terms are computed by iterative solution of Equation (3) [29]. The required integrals over the Fermi surface are evaluated using a modified tetrahedron method [30]. These calculations were designed to be fully quantitative within the limitations of the LDA and muffin-tin models. The results most relevant to GMR are those for $3d/4s/4p$ transition and noble metals. For atomic impurities Fe through Zn in Ni, the majority-spin conductivity is very little affected by impurity scattering, while large effects are found for minority-spin conductivity. This implies that scattering by an isolated impurity atom in this series is strongly spin-selective. Similar calculations were carried out for ternary alloys [94].

Calculations using this methodology to study GMR were carried out for FeCr multilayers [77, 78]. Spin-dependent residual resistivities were computed for transition and noble-metal impurities in bcc Fe, using the methods applied earlier. In agreement with qualitative ideas drawn from comparison of band structures for the elemental metals, an interesting reversal of spin-dependent effects is found for impurity atoms that respectively precede and follow Fe in the periodic table. Comparing Cr with Ni, both in Fe, the former shows strong impurity scattering of majority electrons, while the latter shows strong scattering of minority electrons, as in the case of CuCo discussed above. For Co in Fe, electrons of neither spin are strongly scattered. This spin-selective scattering effect was examined in calculations of magnetoresistance for FeCr multilayers. Self-consistent LDA calculations were carried out for a series of layered materials with a superlattice unit cell of composition Fe_3Cr_n with $n = 2$, 12 for parallel magnetization vectors, twice as large for antiparallel magnetization. The layered structure is described by a (100) tetragonal unit cell on the fcc Fe lattice. The Boltzmann equation was used to model impurity scattering by a concentration c of Cr atoms in the Fe layers. An averaged relaxation time computed from the T-matrices obtained in calculations on Cr impurity scatterers in Fe was assigned to all Bloch states of majority spin, and a corresponding averaged parameter value was assigned to all states of minority spin. The ratio of these parameters is the spin asymmetry ratio as obtained in calculations of residual resistivity. Large GMR ratios were found in these calculations, which omitted all scattering mechanisms other than the Cr impurity scattering that was modeled. As a function of spacer layer thickness, the computed GMR showed oscillations described by the authors as quantum coherence oscillations due to the supercell geometry. Because the conductivity tensor is computed directly in the Boltzmann formalism, results were obtained for both CIP and CPP geometries. The latter values of the GMR ratio are larger for all spacer thicknesses, by approximately a factor of 4. Similar calculations using spin-independent relaxation times gave much smaller GMR ratios, consistent with other models based solely on Fermi-surface effects [97]. From the residual resistivity studies, it is expected that Cr and Cu atoms as scattering centers in Fe should have opposite spin-dependent effects. This was studied by Zahn et al. [78]. The combination of both impurities was found to reduce the computed GMR ratio significantly. An effect of this kind has been observed as inverse spin-valve magnetoresistance [10].

All three of the methods cited above that have been used for *ab initio* calculations of the electronic structure of GMR materials are versions of multiple-scattering theory. In this theory, local solutions of the LDA Schrödinger equation are computed by numerical integration in each atomic cell or sphere and then combined into solutions that satisfy global continuity and boundary conditions. Solutions corresponding to poles of the Green's function exist at energy values $\epsilon(s, \mathbf{k})$ determined by the secular equation

$$\det(\mathbf{I} - \mathbf{gt}) = 0. \tag{19}$$

Here $\mathbf{t}(\epsilon)$ is an atomic-cell scattering matrix and $\mathbf{g}(\epsilon, \mathbf{k})$ is a matrix of structure constants. Matrix t is constructed from local solutions of the Schrödinger equation, while $\mathbf{g}$ is a matrix representation of the free-electron Green's

function for a given geometrical structure. The energy bands of magnetic and spacer metals in typical layered GMR materials match closely at the Fermi energy in one spin direction, while there is a substantial mismatch for the opposite spin [87]. Because energy bands in a fixed-space lattice are determined entirely by the t-matrices, the spin-dependent t-matrices of the two atomic species at the Fermi energy must also be very similar for one spin direction and different for the other. This observation immediately implies a possible mechanism for enhanced magnetoresistance [79]: If these two species interdiffuse across a layer boundary in a magnetized material, the resultant impurity scattering is determined by the difference Δt of the spin-dependent t-matrices. This will be large for one spin direction and small for the other, which implies spin-dependent dissipative scattering for random interpenetration of the adjacent metals. This in turn implies magnetoresistance. Since this scattering mechanism must be concentrated at layer interfaces or grain boundaries, it is consistent with the strong interfacial spin-dependent scattering effect deduced from experimental data and parametric theories. The question to be resolved is whether the magnitude of resistivity due to this scattering mechanism is large enough to make a significant contribution to observed GMR ratios. Calculations designed to examine this question were carried out on superlattice models of layered CuCo [79] and CrFe [98, 99]. The answer was found to be clearly affirmative, in qualitative agreement with the large GMR effects found in calculations by Butler et al. [76, 88] and by Zahn et al. [78]. The general conclusion of these *ab initio* studies is that this is in fact the dominant mechanism for the observed GMR.

In the LACO method, as used for *ab initio* GMR calculations, multiple-scattering theory is expressed in terms of t-matrices computed for space-filling local atomic (Wigner–Seitz) cells. This allows a more direct treatment of the outer region of each atom than does the muffin-tin approximation, used for example in LKKR calculations. In the reported study of layered CuCo, preliminary self-consistent calculations on fcc Cu and on both paramagnetic and ferromagnetic Co (on the fcc Cu lattice) provided initial radial density functions for (001)-tetragonal (CuCoCu)(CuCoCu), also on the fcc Cu space lattice. This defines the supercell of a layered model system in which the magnetization of successive Co planes can be set either parallel ($\uparrow\uparrow$) or antiparallel ($\uparrow\downarrow$). Self-consistent calculations were carried to convergence for both magnetization alignments using an energy-dependent basis set designated by spd(fg) for each atomic cell [81]. These calculations provided the raw data needed for perturbation theory computations of point-to-point scattering rates over the Fermi surface due to a concentration c of impurity atoms Cu in Co (hence concentration $c/2$ of interchanged Co atoms in each Cu layer) due to diffusion across the CoCu interface [79]. The calculations assumed that spin polarization was preserved for the displaced atoms and their neighbors, and simplified the scattering problem by neglecting Green's-function corrections to the bare scattering matrix Δt and by omitting scattering-in corrections. All results given here are internally consistent, but numbers differ from the original CuCo publication [79] because of some program upgrades and a redefinition of c.

Retaining impurity concentration c as an unknown parameter, calculations in the sparse impurity limit give relaxation times in the form $c\tau$ for each Bloch wave state at the Fermi level. The results show large spin dependence and large variation with magnetization alignment. The computed values, in atomic units, differ by orders of magnitude:

$$\uparrow\uparrow(f) \quad c\tau(\uparrow) \simeq 10^4 \quad c\tau(\downarrow) \simeq 10^1;$$

$$\uparrow\downarrow(a) \quad c\tau(\uparrow) \simeq 10^2 \quad c\tau(\downarrow) \simeq 10^2.$$

The resulting conductivity tensor is strongly spin-dependent. The computed in-plane conductivities (CIP) are, in atomic units,

$$\uparrow\uparrow(f) \quad c\sigma(\uparrow) = 0.53096 \quad c\sigma(\downarrow) = 0.00068$$
$$c\sigma(f) = 0.53163;$$

$$\uparrow\downarrow(a) \quad c\sigma(\uparrow) = 0.00668 \quad c\sigma(\downarrow) = 0.00668$$
$$c\sigma(a) = 0.01336.$$

If this were the only dissipative scattering mechanism at work, the implied magnetoresistance ratio, defined here by $[\sigma(f) - \sigma(a)]/\sigma(a)$, would be the very large factor 38.79. LKKR calculations [76] of spin-dependent scattering due to atomic diffusion in Cu/Co/Cu gave GMR ratios of similar magnitude. The results given above for spin-dependent scattering include the Mott final-state effect. In order to evaluate its contribution to GMR, calculations were carried out with the same spin-dependent transition probabilities, but these were averaged over initial state and spin. Explicitly, in the general formula $\tau^{-1}_{k,\text{out}} = \Sigma_{k'} P_{k',k}$ for the quasiparticle lifetime, evaluated at each quadrature grid point on the spin-dependent Fermi surface, the summation symbol includes the spin-dependent density of final states. If the transition probabilities P are averaged over initial states, the computed lifetime τ depends only on the mean density of final states of given spin and models the spin-dependent Mott effect. The modified values of $c\sigma$ computed in this way are

$$\uparrow\uparrow(f) \quad c\sigma(\uparrow) = 0.00863 \quad c\sigma(\downarrow) = 0.00053$$
$$c\sigma(f) = 0.00916;$$

$$\uparrow\downarrow(a) \quad c\sigma(\uparrow) = 0.00057 \quad c\sigma(\downarrow) = 0.00057$$
$$c\sigma(a) = 0.00114.$$

The implied magnetoresistance ratio is 7.04. Hence, the Mott effect by itself can produce enhanced magnetoresistance, but the specific effect of spin-dependent interface scattering gives much larger GMR.

These very large magnetoresistance ratios are valid only in the absence of dissipative scattering by other mechanisms. The observed ratios combine this specific interface scattering effect with the bulk resistivity of the pure metals. Under experimental conditions, mean free paths in the nominally pure metals are by no means infinite. Using estimates of $\lambda(\mathrm{Cu}) = 200$ Å and $\lambda(\mathrm{Co}) = 70$ Å, and weighting $1/\lambda$ for each species by the relative number of atoms in the supercell, the resulting spin-averaged mean free path is given by $1/\lambda = (n_{\mathrm{Cu}}/\lambda_{\mathrm{Cu}} + n_{\mathrm{Co}}/\lambda_{\mathrm{Co}})/(n_{\mathrm{Cu}} + n_{\mathrm{Co}})$. Bulk scattering was modeled by substituting this value of scalar λ into Equation (5). The implied values of σ for spin-independent bulk scattering are

$$\uparrow\uparrow(f) \quad \sigma(\uparrow) = 0.41071 \quad \sigma(\downarrow) = 0.38671$$
$$\sigma(f) = 0.79741;$$
$$\uparrow\downarrow(a) \quad \sigma(\uparrow) = 0.47604 \quad \sigma(\downarrow) = 0.47604$$
$$\sigma(a) = 0.95209.$$

The implied magnetoresistance ratio for spin-independent bulk scattering is -0.16, opposite in sign from the observed GMR, if spin-dependent impurity scattering is neglected. This result indicates that despite the spin dependence of the Fermi surface, purely spin-independent scattering cannot account for GMR. For comparison with observed data, resistivities due to bulk scattering and to spin-dependent interface scattering must be combined. Resistivities are added separately for each spin; then the resulting spin-indexed conductivities are added. This gives a rational function of interpenetration concentration c that interpolates $\Delta R/R$ between pure bulk and interface scattering limits. If c is taken to be 0.05, and other quantities are taken from the data given above, this formula gives $\Delta R/R \simeq 0.96$, which is comparable to estimates of the empirical limit of GMR values for this extreme example of single atomic layers.

These superlattice calculations obtain similar results for the perpendicular principal axis of the conductivity tensor, relevant to CPP geometry if the local electric field can be averaged over the tetragonal translational unit cell of this model. From the Fermi surface and relaxation times used above for CIP geometry, the corresponding results for $c\sigma_{zz}$ due to atomic interdiffusion in the model superlattice (CuCoCu)(CuCoCu) are

$$\uparrow\uparrow(f) \quad c\sigma(\uparrow) = 2.15654 \quad c\sigma(\downarrow) = 0.00291$$
$$c\sigma(f) = 2.15946;$$
$$\uparrow\downarrow(a) \quad c\sigma(\uparrow) = 0.00480 \quad c\sigma(\downarrow) = 0.00480$$
$$c\sigma(a) = 0.00961.$$

The implied value of $\Delta R/R$ is 223.7. However, the computed magnetoresistance ratio for pure bulk scattering, parametrized as above, is 0.24. When these physical mechanisms are combined for $c = 0.05$, the value of $\Delta R/R$ is 6.63, significantly larger than the CIP ratio but of the same order of magnitude.

Similar calculations have been reported for layered CrFe, modeled as a superlattice with (001) tetragonal unit cell (CrFeCr)(CrFeCr) on the bcc Fe space lattice [98, 99]. Here a point of particular interest is the expected reversal of the spin-sense of the polarized current flow [79], compared with the favored majority spin current flow in CuCo. The mechanism is shown very clearly in the essentially quantitative calculation of impurity scattering in Fe by Mertig et al. [77]. These authors find that residual resistivities for majority carriers are much larger than for minority carriers for Cr in Fe, whereas the opposite is true for Cu in Co, from the calculations discussed above [76, 79] and from unpublished results by Mertig [100] based on impurity calculations by Stepanyuk et al. [96]. Superlattice calculations on layered CrFe [99] give values of in-plane $c\sigma$ for the atomic interpenetration mechanism as

$$\uparrow\uparrow(f) \quad c\sigma(\uparrow) = 0.00032 \quad c\sigma(\downarrow) = 0.01632$$
$$c\sigma(f) = 0.01664;$$
$$\uparrow\downarrow(a) \quad c\sigma(\uparrow) = 0.00186 \quad c\sigma(\downarrow) = 0.00186$$
$$c\sigma(a) = 0.00372.$$

In contrast to CuCo, the conductivity here is dominated by electrons of minority spin. If there are no transitions by other scattering mechanisms, the implied magnetoresistance ratio is 3.47.

Modeling the pure Mott effect, as discussed above for CuCo, gives $\Delta R/R = 2.31$. All ratios here are smaller than in the case of layered CuCo, and the Mott final-state effect is relatively more important. When pure bulk scattering is modeled with empirical mean free path values $\lambda = 40$ Å for both Cr and Fe, the magnetoresistance ratio computed from the spin-polarized superlattice energy-band structure is -0.05. When bulk and interface scattering are combined, the rational formula evaluated for $c = 0.05$ gives $\Delta R/R \simeq 1.07$, consistent with estimates of the experimental limit for the extreme case of single atomic layers. These calculations [98, 99] included results (not published) for CPP geometry, assuming that the local electric field can be averaged over the (CrFeCr)(CrFeCr) translational cell. As in the case of layered CuCo, all ratios are found to be larger for CPP geometry than for CIP geometry. The CPP magnetization ratio for spin-dependent interface scattering alone is computed to be

6.06, reduced to 2.11 for the pure Mott effect, and −0.18 for pure bulk scattering. Combining bulk and interface scattering for interpenetration concentration $c = 0.05$ gives $\Delta R/R \simeq 1.26$, greater than the CIP ratio but by a smaller factor than that found for layered CuCo.

These calculations show the expected reversal of the spin sense of the steady-state polarized electronic current density, determined by spin-dependent dissipative scattering due to interchange of atoms of two species across an interface. Since this effect is governed by the self-consistent t-matrices computed for these atoms in their metallic environments, it is appropriate to characterize this as an atomic mechanism, which appears to be the principal underlying cause of GMR. By implication, an electronic current passing through a magnetized magnetic/spacer interface is spin-polarized to the extent that the spin-indexed atomic t-matrices differ at the Fermi energy. A second interface of this kind placed within a spin diffusion length (determined by spin-flip scattering or precession in a magnetic field) will act as a polarization analyzer. If such a combination of polarizer and analyzer could be realized experimentally, it would constitute a micromagnetometer or magnetoelectric switching device [98, 99]. A simple test of these ideas is to fabricate a device with like interface elements, which should show a resistance minimum for parallel-aligned magnetization vectors, and compare with unlike interface pair elements like CuCo and CrFe in the same structure, for which the resistance should be maximized by parallel magnetization. This has been realized to some extent in a recent experiment showing inverse GMR [10], and discussed by Zahn et al. [78] as a consequence of the opposite spin sense for residual resistivity due to Cr and Cu impurities, respectively, in Fe.

The *ab initio* calculations support the conclusion that spin-dependent interface scattering is decisive for the largest observed GMR ratios. However, it is clear that the Mott final-state effect implies spin-dependence for any generic scattering mechanism (which may itself be independent of spin) in the bulk of a magnetized transition metal or alloy. The calculations by Nesbet [79, 99] show that relatively large GMR can result from the Mott effect alone, when state-to-state scattering probabilities are spin-averaged. Since these calculations model atomic layers that are all located at an interface, they do not give specific information about bulk scattering. It is relevant here that the spin asymmetry ratios α from *ab initio* calculations compiled and summarized by Mertig [100] in general are different if host and impurity species are interchanged. For example, α for Co in Ni is 92.4, while α for Ni in Co is 522.4. A simplified explanation of this difference is that the spin asymmetry parameter is determined both by the difference of atomic-cell t-matrices, which would give equivalent effects if two species with similar band structure at the Fermi level were interchanged, and by the Mott effect, which is characteristic of the energy-band structure of the host species, hence different in the two cases. The simplest conclusion is that the two values of α are large because of large Δt, but that they differ because of the Mott effect for the different host metals. The computed value of α for Fe in Ni is very large (an experimental value is 20 [43]), while that for Ni in Fe is 5.48 (experimental value 3 [43]). Although different values of α might be expected because of the different lattice structures of hosts fcc Ni and bcc Fe, the difference between Co in Ni and Ni in Co must be due to the detailed band structure and minority-band occupancy. In CPA theory, Δt is defined for each atom as the difference between its atomic-cell t-matrix and the statistical t-matrix of the coherent potential. Including the Mott effect, the large value of α for Fe in Ni implies a substantial bulk scattering spin asymmetry in permalloy, as computed in the *ab initio* CPA calculations of Butler et al. [76, 89, 91]. Taking into account the very large values of α for Co in Ni or Ni in Co, this is not inconsistent with the experimental data of Parkin [11], which show that the interface effect of a thin Co layer in permalloy dominates any bulk scattering effect on GMR. It is interesting to note that the parametric model study by Dieny [49] of Py/Cu spin-valve structures finds $\lambda_{\downarrow} = 6$ Å, indicating that the minority-spin resistivity is high and minority-spin current density is low even in a model of permalloy that includes only bulk scattering parameters.

Summary and conclusions

This paper has reviewed theoretical models of spin-dependent scattering in GMR materials. Experimental data indicate that the magnitude of GMR in layered materials is controlled primarily by some mechanism associated with magnetic/spacer interfaces. Parametrized semiclassical and quantum-theoretical models of spin-polarized electron transport identify the parameters relevant to this interface effect, emphasizing the spin asymmetry α for impurities implanted in transition metals. The interface effect is modeled in terms of spin-dependent impurity scattering concentrated in an interface layer of atomic dimensions. Recent *ab initio* calculations of the spin-dependent energy-band structure and of the resulting spin-dependent conductivity provide quantitative values of the spin asymmetry ratio and demonstrate its relevancy to GMR materials. These *ab initio* calculations study the specific mechanism of spin-selective scattering by transition-metal atoms embedded in a nonmagnetic substrate or of nonmagnetic atoms embedded in a transition-metal substrate, and of atoms displaced across the boundaries of magnetized layers or granules. This essentially atomic mechanism appears to be the principal cause of the observed GMR in Fe/Cr and Co/Cu

materials. These calculations include the basic mechanism for spin-dependent scattering proposed by Mott, a consequence of spin-polarized energy-band structure in transition metals, which is omitted in parametric models based on free-electron energy bands. The Mott effect causes any generic scattering mechanism to be spin-dependent in a magnetized transition metal and augments the effect of spin-dependent interface scattering in GMR materials. In the CPA model of a substitutional alloy, each atom is surrounded by a statistical distribution of neighbors. This implies that both Mott and atomic interdiffusion effects are present in the interior of a magnetic alloy. A parametrized model finds a very short mean free path for minority-spin electrons in permalloy, and *ab initio* calculations indicate significant spin-dependent bulk scattering.

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